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On Discretization and Differentiation
of Operators
with Application to Newton's Method
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ABSTRACT

In the numerical solution of operator equations $Fx = 0$, discretization of the equation and then application of Newton's method results in the same linear algebraic systems of equations as application of Newton's method followed by discretization. This leads to the general problem of determining when the two frequently used operations of discretization and (Frechet) differentiation applied to a non-linear operator are commutative. A theory of discretization processes is developed here which proves that for a wide class of operators of interest in applications, discretization and differentiation indeed "commute". The fundamental concept of the theory is a distinction between the discretization of the linear spaces involved and the replacement of the infinitesimal parts of the operator F, i.e., those parts involving, e.g., differentiation and integration, by a discrete analogue. Using this distinction in an abstract way a "complete" discretization process is defined precisely and the cited commutativity results are proven. The results are then applied to Newton's method.

CONTENTS

On Discretization and Differentiation of Operators

with Application to Newton's Method

by James M. Ortega and Werner C. Rheinboldt

1. **Introduction.**

Let

(1) $$F(x) = 0$$

represent a non-linear integral or differential equation. A common

approach to the approximation of a solution of (1) is the following

(see, e.g., Collatz [1]): First, discretize (1), that is, associate

with x a vector $\bar{x} \in R^n$ whose components approximate x at n (grid)

points, and then replace integrals by quadrature sums and deriva-

tives by difference quotients involving only the components of $\bar{x}$.

As a result of this discretization, (1) is replaced by a system of

n nonlinear equations in n unknowns:

(2) $$\bar{F}(\bar{x}) = 0.$$

Assume now that this system can be solved by Newton's method,

and introduce the "Newton"-function

(3) $$\bar{N}(\bar{x}, \bar{y}) = \bar{F}'(\bar{x})\bar{y} + \bar{F}(\bar{x}),$$

where $\bar{F}'(\bar{x})$ is the Frechet-derivative (Jacobian matrix) of $\bar{F}$ at $\bar{x}$.

If $\bar{x}$ is an approximation to a solution of (2) then a correction $\bar{y}$

to $\bar{x}$ is computed as the solution of the linear algebraic system

(4) $$\bar{N}(\bar{x}, \bar{y}) = 0.$$

Alternately, it may be possible to apply the (generalized)

Newton method directly to (1) (see, e.g., Kantorovich [2] or Kantorovich and Akilov [3]). Then, of course, the Newton correction y to an approximate solution x of (1) is obtained as a solution of the linear operator equation

$$(5) \qquad N(x,y) \equiv F'(x)y + F(x) = 0.$$

If F(x) = 0 represents, for example, an integral equation, (5) is an integral equation for y. In general, it is necessary to apply approximation methods to solve this linear operator equation, and if (5) is discretized there results again a system of linear algebraic equations:

$$(6) \qquad \tilde{N}(\tilde{x},\tilde{y}) = 0.$$

A natural question is now the following. Is it better, in some still to be specified sense, to discretize first and then apply Newton's method, or, rather, to apply Newton's method first and then discretize? An answer to this question involves many aspects, such as the ease of obtaining discretization error bounds, and our concern here is only with the following observation: Under certain rather general conditions it turns out that the equations (4) and (6) are identical, provided the discretizations are carried out in the same way. In other words, as far as the final linear algebraic equations are concerned, it makes no difference whether Newton or discretization is applied first; loosely speaking, Newton and discretization "commute". However, a little reflection shows that this observation concerns Newton's method only incidentally,

and that basically the central question is when the operations of discretization and differentiation "commute".

In Section 2 we shall describe a general setting for an investigation of this commutativity question and give in detail two concrete examples. In Section 3 we present a complete answer for a certain limited class of operators, and ,in Section 4, this in turn will be the basis for an extension of the theory to classes of operators that are of interest in applications. Finally, in Section 5 we return to Newton's method as an example of the application of our results; this will make precise the discussion in this introduction.

2. Notation and Examples

Throughout this paper, X, Y, etc. shall always denote real or complex Banach spaces, and $E(X,Y)$ shall be the usual Banach space of all bounded linear operators with domain X and range Y. We shall let $Q(X,Y)$ denote the collection of all mappings $F:D(F) \subset X \to Y$ with a non-empty domain $D(F)$ in X and range in Y. As usual $F \in Q(X,Y)$ shall be called Frechet differentiable at an <u>interior</u> point $x \in D(F)$ if there exists a bounded linear operator $F'(x) \in E(X,Y)$ such that

$$\lim_{\|h\| \to 0} \frac{1}{\|h\|} \| F(x+h) - F(x) - F'(x)h\| = 0.$$

In our discussion it will frequently be necessary to stress that F' is a function of two variables, and accordingly, we shall use the notation $F'(x_1;x_2)$ and $F'(x_1)x_2$ interchangeably. If we define $D'(F) \subset D(F)$ to be the set of all interior points $x \in D(F)$ at which $F'(x)$ exists, then $F' \in Q(X \times X, Y)$ and has domain $D(F') = D'(F) \times X$.

More generally, we can introduce the sets $D^{(k)}(F)$ $(k=1,2,\ldots)$ of all interior points of $D(F)$ at which the kth derivative $F^{(k)}$ exists. Then $F^{(k)}$ is an element of $Q(X^{k+1},Y)$ with domain $D(F^{(k)}) = D^{(k)}(F) \times X^k$, where X^k denotes the product space $X \times X \times \ldots \times X$ (k times). Finally, we denote by $Q'(X,Y)$ the set of all operators $F \in Q(X,Y)$ such that $D'(F)$ is not empty.

Before proceeding with our general development in the next section, we give in the remainder of this section two concrete examples that will illustrate the commutativity of discretization and differentiation.

<u>Example 1:</u> Set $X = Y = C[0,1]$ and let $F:D(F) \subset X \to Y$ be the integral operator

$$(7) \qquad (Fx)(s) = f(s,x(s)) + \int_0^1 g(s,t,x(t))dt.$$

Here the real-valued function f of the two variables s and x, together with its partial derivatives $f_2 \equiv \dfrac{\partial f}{\partial x}$ and $f_{22} \equiv \dfrac{\partial^2 f}{\partial x^2}$, is assumed to be defined and continuous on some open domain $D(f) \subset R^2$, and similarly g, together with g_3 and g_{33} shall be defined and continuous on the open set $D(g) \subset R^3$. Then

$$D(F) = D'(F) = \left\{ x \in C[0,1] \mid (s,x(s)) \in D(f),\ (s,t,x(t)) \in D(g),\ 0 \leq s,t \leq 1 \right\}.$$

In particular, if $D(f)=[0,1] \times (-\infty,+\infty)$ and $D(g)=[0,1] \times [0,1] \times (-\infty,+\infty)$ then $D(F) = D'(F) = C[0,1]$. For $x \in D'(F)$ and $h \in X$, $F'(x;h)$ is given by

$$(8) \qquad (F'(x;h))(s) = f_2(s,x(s))h(s) + \int_0^1 g_3(s,t,x(t))h(t)dt.$$

We choose grid points $0 \leqq s, < \ldots < s_n \leqq 1$, $t_i = s_i$ $(i=1,..,n)$ and quadrature

weights α_j $(j=1,..,n)$ and take as discrete analogues of (7) and (8),

$$(9) \qquad f(s_i, x(s_i)) + \sum_{j=1}^{n} \alpha_j g(s_i, t_j, x(t_j)), \quad (i=1,\ldots,n),$$

and

$$(10) \qquad f_2(s_i, x(s_i))h(s_i) + \sum_{j=1}^{n} \alpha_j g_3(s_i, t_j, x(t_j))h(t_j), \quad (i=1,..,n).$$

Now consider $\bar{X} = R^n$ and the operator $\bar{F}:D(\bar{F}) \subset \bar{X} \to \bar{X}$ defined by

$$(11) \qquad (\bar{F}\bar{x})_i = f(s_i, \bar{x}_i) + \sum_{j=1}^{n} \alpha_j g(s_i, t_j, \bar{x}_j), \quad (i=1,\ldots,n).$$

It is clear that

$$D(\bar{F}) = D'(\bar{F}) = \left\{ \bar{x} \in R^n \mid (s_i, \bar{x}_i) \in D(f), \ (s_i, t_j, \bar{x}_j) \in D(g), \ i,j=1,\ldots,n \right\},$$

and for $\bar{x} \in D'(\bar{F})$ we find that

$$(12) \qquad (\bar{F}'(\bar{x};\bar{h}))_i = f_2(s_i, \bar{x}_i)h_i + \sum_{j=1}^{n} \alpha_j g_3(s_i, t_j, \bar{x}_j)\bar{h}_j, \quad (i=1,..,n).$$

Hence, under the correspondence $x(s_i) = \bar{x}_i$, $h(s_i) = \bar{h}_i$ $(i=1,\ldots,n)$,

we see that (9) and (11), as well as (10) and (12) are identical.

In other words, the discretized form of F' and the derivative of the

discretized operator $\bar{F}$ are the same.

Proceeding in an analogous manner, it is easy to see that the

same result holds for integral operators in several variables, e.g.,

$$(Fx)(s,t) = f(s,t,x(s,t)) + \int_0^1 \int_0^1 g(s,t,\xi,\eta,x(\xi,\eta))d\xi d\eta.$$

Example 2: As usual, let $X = C^2[0,1]$ denote the Banach space of all

twice continuously differentiable real-valued functions on $[0,1]$

with the norm

$$\|x\| = \max\left[\sup_{0\leq t\leq 1} |x(t)|, \quad \sup_{0\leq t\leq 1} |x'(t)|, \quad \sup_{0\leq t\leq 1} |x''(t)| \right].$$

Let $Y = C[0,1]$ and define the differential operator $F:D(F) \subset X \to Y$ by

(13) $\qquad (Fx)(s) = f(s,x(s),x''(s))$, $s \in [0,1]$,

where $f:D(f) \subset R^3 \to R$, together with its partial derivatives f_2, f_{22}, f_3, f_{23}, f_{33}, is assumed to be defined and continuous on the open set $D(f) \subset R^3$.

If we take

$D(F) = D'(F) = \left\{ x \in X \mid (s,x(s),x''(s)) \in D(f), \ 0\leq s\leq 1, \ x(0)=x(1)=0 \right\}$

then clearly for $x \in D'(F)$,

(14) $F'(x;h)(s) = f_2(s,x(s),x''(s))h(s) + f_3(s,x(s),x''(s))h''(s)$.

Set $\Delta = 1/(n+1), s_i = i\Delta$ $(i=0,1,\ldots,n+1)$ and

$$(\delta^2 x)(s_i) = \frac{1}{\Delta^2}\left[x(s_{i+1})-2x(s_i)+x(s_{i-1}) \right], \quad (i=1,\ldots,n),$$

and take as the discrete analogues of (13) and (14)

(15) $\qquad f(s_i, x(s_i), (\delta^2 x)(s_i))$, $(i=1,\ldots,n)$,

and

(16) $\quad f_2(s_i,x(s_i),(\delta^2 x)(s_i))h(s_i) + f_3(s_i,x(s_i),(\delta^2 x)(s_i))(\delta^2 h)(s_i)$.

Now define the discretized operator $\bar{F}:D(\bar{F}) \subset \bar{X} \to \bar{X}, (\bar{X} = R^n)$, by

(17) $\qquad (\bar{F}\bar{x})_i = f(s_i,\bar{x}_i,\delta^2\bar{x}_i)$, $i=1,\ldots,n)$,

where

$$\delta^2\bar{x}_i = \frac{1}{\Delta^2}\left[\bar{x}_{i+1} - 2\bar{x}_i + \bar{x}_{i-1} \right], \quad (i=1,\ldots,n),$$

and

$$D(\bar{F}) = D'(\bar{F}) = \left\{ \bar{x} \in R^n \mid (s, \bar{x}_i, \delta^2 \bar{x}_i) \in D(f), \ i=1, \ldots, n, \ \bar{x}_0 = \bar{x}_{n+1} = 0 \right\}.$$

Then for $\bar{x} \in D'(\bar{F})$ and $i=1, \ldots, n$

$$(18) \qquad (\bar{F}'(\bar{x}; \bar{h}))_i = f_2(s_i, \bar{x}_i, \delta^2 \bar{x}_i) \bar{h}_i + f_3(s_i, \bar{x}_i, \delta^2 \bar{x}_i) \delta^2 \bar{h}_i,$$

and again under the correspondence $x(s_i) = \bar{x}_i$ $(i=0,1,\ldots,n+1)$ we

see that (16) and (18) are identical.

This result also holds for more general ordinary and partial

differential operators as, for example,

$$(19) \qquad (Fx)(s) = f(s, x(s), x'(s), \ldots, x^{(m)}(s)),$$

and

$$(20) \qquad (Fx)(s,t) = f(s, t, x(s,t), \frac{\partial x}{\partial s}(s,t), \ldots, \frac{\partial^m x}{\partial s^m}(s,t)),$$

and - when combining the results of Examples 1 and 2 - also for

integro-differential operators, such as

$$(21) \quad (Fx)(s) = f(s, x(s), \ldots, x^{(m)}(s)) + \int_0^1 g(s, t, x(t), \ldots, x^{(m)}(t)) dt.$$

3. Space Discretization and Induced Operator Discretization

In order to begin the general discussion of our commutativity

question posed in the previous two sections, let us consider the

following setting for the discretization:

Let X and Y be two Banach spaces and assume that two other

Banach spaces $\bar{X}$ and $\bar{Y}$ represent discretized versions of X and Y,

respectively. Usually $\bar{X}$ and $\bar{Y}$ are finite-dimensional, but here

we do not assume this. The spaces X and $\bar{X}$, and similarly Y and $\bar{Y}$,

are assumed to be connected by "discretization mappings $\varphi \in E(X, \bar{X})$

and $\psi \in E(Y, \overline{Y})$ with the property that $\varphi X = \overline{X}$ and $\psi Y = \overline{Y}$.

It is usual in theoretical investigations of discretization to consider some fixed operator $F \in Q(X,Y)$, together with a "discretized" operator $\overline{F} \in Q(\overline{X}, \overline{Y})$ and to assume that $\overline{F}$ is "close" to F in some sense. For example, Kantorovich [2] assumes that

$$\|F(\varphi x) - \psi(Fx)\| \leq \epsilon \|x\|, \quad x \in D(F).$$

Here we will not be concerned with the "approximation" of F by $\overline{F}$, but our interest is rather in the formal structure of the discretization process itself.

The discretization of operators such as those of Examples 1 and 2, involves of course not only the replacement of the spaces X and Y by $\overline{X}$ and $\overline{Y}$, but more importantly, the replacement of the operations of integration and differentiation by their discrete analogues. We shall postpone to Section 4 any consideration of these latter replacements and we shall consider in this section only the following very special class of operators.

<u>Definition 1.</u> Let the mappings $\varphi_k \in E(X^k, \overline{X}^k)$, $(k=1,2,\ldots)$ be defined by

$$\varphi_k(x_1,\ldots,x_k) = (\varphi x_1, \varphi x_2, \ldots, \varphi x_k).$$

Then if $G \in Q(X^k, Y)$, we say that G is <u>discretization-compatible</u> (or <u>d-compatible</u> for short), and write $G \in D(\Phi_k)$, if $\varphi_k u = \varphi_k v$ for u, v $\in D(G)$ implies that $\psi(Gu) = \psi(Gv)$.

We note that in Example 1 we have $\overline{X} = \overline{Y} = R^n$ and

$$\varphi(x) \equiv \psi(x) = (x(s_1),\ldots,x(s_n)).$$

Of course the operator F of (7) is in general not d-compatible, since this would mean that $u(s_i) = v(s_i)$, i=1,...,n, implies that

$$f(s_i, u(s_i)) + \int_0^1 g(s_i, t, u(t))dt = f(s_i, v(s_i)) + \int_0^1 g(s_i, t, v(t))dt.$$

Note, however, that for $g \equiv 0$ the operator F is trivially d-compatible. Moreover, if in this case $\psi(x) = (x(t_1), \ldots, x(t_n))$ is chosen independently of φ, then F is d-compatible if and only if $m = n$ and $t_i = s_i$ (i=1,...,n), i.e., if and only if $\varphi \equiv \psi$.

Now for each $G \in D(\Phi_k)$, the operator

$$(22) \quad \bar{G}:D(\bar{G}) = \varphi_k(D(G)) \subset \bar{X}^k \rightarrow \bar{Y}, \quad \bar{G}\bar{x} = \psi(Gx), \quad \bar{x} = \varphi_k x, \quad x \in D(G),$$

is well-defined and we have a natural association of operators in $D(\Phi_k)$ with certain operators in $Q(\bar{X}^k, \bar{Y})$. That is, the space discretizations φ_k and ψ induce "operator discretizations" in the class $D(\Phi_k)$.

<u>Definition 2.</u> The mapping

$$(23) \quad \Phi_k:D(\Phi_k) \subset Q(X^k, Y) \rightarrow Q(\bar{X}^k, \bar{Y}), \quad \Phi_k G = \bar{G}, \quad D(\bar{G}) = \varphi_k(D(G))$$

where $\bar{G}$ is given by (22), shall be called an <u>operator discretiza-tion mapping</u> and $\bar{G}$ shall be called a Φ-<u>discretization</u> of G.

In principle, these definitions are statements about quotient mappings: Define $N(\varphi_k) = \left\{ x \in X^k \mid \varphi_k x = 0 \right\}$, $N(\psi) = \left\{ y \in Y \mid \psi y = 0 \right\}$, and let $\hat{X}^k = X^k/N(\varphi_k)$, $\hat{Y} = Y/N(\psi)$ denote the quotient spaces. Then $G \in D(\Phi_k)$ assures the existence of a quotient mapping

$$\hat{G}:D(\bar{G})/N(\varphi_k) \subset \hat{X}^k \rightarrow \hat{Y}.$$

But, $\hat{X}^k$ and $\bar{X}^k$ as well as $\hat{Y}$ and $\bar{Y}$ are linearly homoemorphic; hence

G induces in the natural way a mapping from $\bar{X}^k$ into $\bar{Y}$, and this

mapping is just the Φ-discretization $\bar{G}$ of G.

In line with this, the following lemma, proven here for complete-

ness, is in essence a well-known result in the theory of quotient

mappings. Its content is that if G is a bounded linear operator in

one of its variables for fixed values of its other variables, then

the same is true of $\Phi_k G$.

Lemma 1: Let $G \in D(\Phi_k)$ and $\bar{G} = \Phi_k G$. If for fixed $x_j \in X$, $j \neq i$,

$$G_i \equiv G(x_1, \ldots, x_{i-1}, \cdot, x_{i+1}, \ldots, x_k) \in E(X,Y), \text{ then}$$

$$L \equiv \bar{G}(\varphi x_1, \ldots, \varphi x_{i-1}, \cdot, \varphi x_{i+1}, \ldots, \varphi x_k) \in E(\bar{X}, \bar{Y}).$$

Proof: The linearity of the operator L is evident; to show that it

is continuous, note first that

$$\|L\varphi x\| = \|(\Phi_k G)(\varphi x_1, \ldots, \varphi x_{i-1}, \varphi x, \varphi x_{i+1}, \ldots, \varphi x_k)\|$$

$$= \|\psi(G(x_1, \ldots, x_{i-1}, x, x_{i+1}, \ldots, x_k))\|$$

$$\leq \|\psi\| \, \|G_i\| \, \|x\|, \quad x \in X,$$

which shows that the linear operator $L\varphi$ from X into $\bar{Y}$ is continuous.

Thus, if S is any open set in $\bar{Y}$, the set $(L\varphi)^{(-1)} S = \varphi^{(-1)}(L^{(-1)} S)$

is open in X. But since φ is linear, continuous and onto $\bar{X}$, it

follows from the interior mapping principle that $L^{(-1)} S$ is open.

Hence, L is continuous and $L \in E(\bar{X}, \bar{Y})$.

For the sake of simplicity we now restrict our attention to the

classes $D(\Phi_1)$ and $D(\Phi_2)$. The following lemma says in essence that

d-compatibility is preserved under differentiation.

Lemma 2: Let $G \in D(\Phi_1) \cap Q'(X,Y)$; then $G' \in D(\Phi_2)$.

Proof: Let $u = (u_1, u_2)$ and $v = (v_1, v_2)$ be in $D(G')$ with $\varphi_2 u = \varphi_2 v$.

Then $u_1, v_1 \in D'(G)$ and for t sufficiently small $u_1 + tu_2$, $v_1 + tv_2 \in D(G)$.

Thus, by definition,

$$G'(u_1, u_2) = \frac{1}{t}[G(u_1 + tu_2) - G(u_1)] + \mathcal{E}_1(t),$$

and

$$G'(v_1, v_2) = \frac{1}{t}[G(v_1 + tv_2) - G(v_1)] + \mathcal{E}_2(t),$$

where $\|\mathcal{E}_i(t)\| \to 0$ for $t \to 0$ $(i=1,2)$. Since $G \in D(\Phi_1)$ and

$$\varphi(u_1 + tu_2) = \varphi(v_1 + tv_2),$$

we then have

$$\psi[G'(u_1, u_2) - G'(v_1, v_2)] = \frac{1}{t}\psi[G(u_1 + tu_2) - G(v_1 + tv_2)] +$$

$$+ \frac{1}{t}\psi[G(u_1) - G(v_1)] + \psi[\mathcal{E}_1(t) - \mathcal{E}_2(t)] = \psi[\mathcal{E}_1(t) - \mathcal{E}_2(t)].$$

Hence,

$$(24) \quad \|\psi[G'(u_1, u_2) - G'(v_1, v_2)]\| \leq \|\psi\|(\|\mathcal{E}_1(t)\| + \|\mathcal{E}_2(t)\|).$$

But the left side of (24) is independent of t while the right

side goes to zero with t. Hence $\psi[G'(u_1, u_2)] = \psi[G'(v_1, v_2)]$, i.e.,

$G' \in D(\Phi_2)$.

The following theorem is the first commutativity result and

the relation (25) is typical of the further results we shall obtain

in the next section.

Theorem 1: Let $G \in D(\Phi_1) \cap Q'(X,Y)$. Then $(\Phi_1 G)'$ is defined on

$D(\Phi_2 G') = \varphi_2(D(G'))$ and

$$(25) \qquad\qquad (\Phi_1 G)' = \Phi_2 G' \quad \text{on } D(\Phi_2 G').$$

Proof: By Lemma 2, $G' \in D(\Phi_2)$ and by definition

$D(\Phi_2 G') = \varphi_2(D(G')) = \varphi(D'(G)) \times X$. Let $x = (x_1, h) \in D(G')$; then

$x_1 \in D'(G) \subset D(G)$. By Lemma 1, $(\Phi_2 G')(\bar{x}_1, \bar{h})$ is a bounded linear

operator in $\bar{h}$ for fixed $\bar{x}_1$, and we have to show that

$$(26) \quad \lim_{\|h\| \to 0} \frac{1}{\|\bar{h}\|} \|(\Phi_1 G)(\bar{x}_1 + \bar{h}) - (\Phi_1 G)(\bar{x}_1) - (\Phi_2 G')(\bar{x}_1, \bar{h})\| = 0$$

where $\bar{x}_1 = \varphi(x_1)$.

Form again the quotient-space

$$\hat{X} = X/N(\varphi_1) = \left\{ \hat{x} \mid \hat{x} = \varphi^{(-1)}(\bar{x}), \ \bar{x} \in \bar{x} \right\}.$$

$\hat{X}$ is a Banachspace under the usual norm $\|\hat{x}\| = \inf[\|x\| \mid x \in \hat{x}]$, and

the induced mapping $\hat{\varphi}: \hat{X} \to \bar{X}$ defined by $\hat{\varphi}(\hat{x}) = \hat{\varphi}(\varphi^{(-1)}(\bar{x})) = \bar{x}$ is

linear, continuous, one-to-one, and onto $\bar{X}$. Hence $\hat{\varphi}$ has a bounded

inverse $\hat{\varphi}^{-1}$ and for any $\bar{h} \in \bar{X}$, $(\bar{h} \neq 0)$ there always exist

$h \in \varphi^{(-1)}(\bar{h}) \subset X$ such that

$$0 < \|\hat{h}\| \leqq \|h\| \leqq 2\|\hat{h}\| \leqq 2\|\hat{\varphi}^{-1}\| \ \|\bar{h}\|.$$

Selecting only such h, we obtain for any $\bar{h} \in \bar{X}$ such that

$\bar{x}_1 + \bar{h} \in D(\Phi_1 G)$,

$$\frac{1}{\|\bar{h}\|} \|(\Phi_1 G)(\varphi(x_1 + h)) - (\Phi_1 G)(\varphi x_1) - (\Phi_2 G')(\varphi x_1, \varphi h)\| =$$

$$= \frac{1}{\|\bar{h}\|} \|\psi[G(x_1 + h)] - \psi[G(x_1)] - \psi[G'(x_1; h)]\| \leqq$$

$$\leqq \frac{2\|\psi\| \ \|\hat{\varphi}^{-1}\|}{\|h\|} \|G(x_1 + h) - G(x_1) - G'(x_1; h)\|.$$

If now $\bar{h} \to 0$, then clearly $h \to 0$ for our choice of $h \in \varphi^{(-1)}(\bar{h})$

and hence the right hand side tends to zero by assumption. This

completes the proof.

It is interesting to note that in general $D((\Phi_1 G)')$ strictly includes $D(\Phi_2 G')$, i.e., $(\Phi_1 G)'$ is an extension of $\Phi_2 G'$. Consider, for instance, the special case of Example 1 when $g \equiv 0$ and $f(s,x) = x^{2/3}$, i.e., $(Fx)(s) \equiv x(s)^{2/3}$. Then

$$D'(F) = \left\{ x \in C[0,1] \mid x(s) \neq 0, 0 \leq s \leq 1 \right\}$$

and therefore

$$D(\Phi_2 F') = \left\{ (\bar{x}_1, \ldots, \bar{x}_n) \mid \bar{x}_i > 0 \text{ or } \bar{x}_i < 0 \text{ for all } i \right\} \times \bar{X}$$

while

$$D((\Phi_1 F)') = \left\{ (\bar{x}_1, \ldots, \bar{x}_n) \mid \bar{x}_i \neq 0, i=1,\ldots,n \right\} \times \bar{X}.$$

Theorem 1 also shows that in essence we have only commutativity between the generic terms "differentiation" and "discretization". Actually just as the discretization operators Φ_1, Φ_2 operate on different classes of functions, the same is true for differentiation. In fact, if we denote differentiation on X and $\bar{X}$ by ∂ and $\bar{\partial}$, respectively, then (25) becomes

$$\bar{\partial}(\Phi_1 G) = \Phi_2(\partial G) \text{ on } D(\Phi_2(\partial G)).$$

It should also be noted that Theorem 1 can be extended to m-times differentiable functions with the result that $(\Phi_1 G)^{(m)} = \Phi_{m+1} G^{(m)}$ on some suitable domain. We omit the details here.

4. Complete Discretization

As mentioned in Section 3, the operators (7) and (13) in Examples 1 and 2 are not in general d-compatible and, moreover, the application of the mapping Φ_1 alone could certainly not be expected to produce the discretized forms (9) and (15). We consider in this section the replacement of the operations of integration and differentiation by discrete analogues and then combine these replacements with the Φ-discretization of Section 2.

We consider first a class of operators corresponding to the case discussed in Example 1. If we introduce there the intermediate Banach space $Z = C([0,1] \times [0,1])$ then the operator F can be considered as a composition of the form $F = KG$ where $G:D(G) \subset X \to Z$ is the operator

$$(27) \qquad (Gx)(s,t) = f(s,x(s)) + g(s,t,x(t)),$$

and $K \in E(Z,Y)$ is the integral operator

$$(28) \qquad (Kz)(s) = \int_0^1 z(s,t)dt.$$

The replacement of integration by quadrature amounts to the replacement of the operator K by another operator $K_d \in E(Z,Y)$ of the form

$$(29) \qquad (K_d z)(s) = \sum_{j=1}^m \alpha_j z(s,t_j).$$

Note that K_d is an operator on the same space as K and not on a discretized space.

Clearly there are many possible operators K_d of the form (29) depending on the choice of the quadrature weights α_j and the grid

points t_j. Whereas usually only those α_j and t_j will be selected,
which assure that K_d is "close" to K, our concern here is with the
formal replacement of K by K_d. What shall be required of K_d is merely
that the operator $F_d = K_d G$ be d-compatible and this is a restriction
only on the grid points t_j. Thus if $\varphi x = \psi x = (x(s_1),...,x(s_n))$,
we choose m = n and $t_j = s_j$, j=1,...,n; then F_d has the form

$$(30) \qquad (F_d x)(s) = f(s,x(s)) + \sum_{j=1}^{n} \alpha_j g(s,t_j,x(t_j)),$$

and a Φ-discretization of F_d gives the final discretized form (9).

Generally for each $K \in E(Z,Y)$ and each positive integer k, we
define the class of operators

$$(31) \quad \mathfrak{F}_k(K) = \left\{ F:D(F) \subset X^k \to Y \mid F=KG,\ G \in Q(X^k,Z),\ D(F)=D(G) \right\}.$$

<u>Definition 3:</u> For any two $K,K_d \in E(Z,Y)$ the mapping

$$(32) \qquad \Psi_k:\mathfrak{F}_k(K) \to \mathfrak{F}_k(K_d), \qquad \Psi_k F \equiv \Psi_k(KG) = K_d G,$$

shall be called a <u>prediscretization mapping</u> for $\mathfrak{F}_k(K)$.

Clearly these mappings Ψ_k have no a-priori relation to dis-
cretization in the usual sense; this would depend on the choice of
the two operators K and K_d. However, the structure of this replace-
ment process corresponds to our intuitive notion of discretization
processes.

The following lemma, an easy consequence of the chain rule,
gives a commutativity result for pre-discretization mappings.

<u>Lemma 3:</u> For given $K,K_d \in E(Z,Y)$ and k = 1,2, let $\Psi_k:\mathfrak{F}_k(K) \to \mathfrak{F}_k(K_d)$

be pre-discretization mappings. If $F = K G \in \mathfrak{F}_1(K)$ and $G \in Q'(X,Z)$

then $F' \in \mathfrak{F}_2(K)$ and $(\Psi_1 F)' = \Psi_2 F'$ on $D(F') = D(G')$.

Proof: By the chain rule we have $D(F') = D(G')$ and $F' = (KG)' = KG'$.

Hence $F' \in \mathfrak{F}_2(K)$ and $\Psi_2 F' = K_d G' = (K_d G)' = (\Psi_1 F)'$ on $D(F')$.

We now combine prediscretization and Φ-discretization.

Definition 4: For given pre-discretization mappings $\Psi_k : \mathfrak{F}_k(K) \to \mathfrak{F}_k(K_d)$

and given Φ-discretization mappings Φ_k as in Definition 2, define

the following subclasses of $\mathfrak{F}_k(K)$:

(33) $\qquad D(\bar{\Psi}_k) = \left\{ F \in \mathfrak{F}_k(K) \mid \Psi_k F \in D(\Phi_k) \right\}, \quad k = 1,2,\ldots \; .$

Each Φ_k is defined on the class $\varphi_k(D(\Psi_k))$ and accordingly let

(34) $\qquad \bar{\mathfrak{F}}_k(K_d) = \left\{ \bar{F} : D(\bar{F}) \subset \bar{X}^k \to \bar{Y} \mid \bar{F} = \Phi_k \Psi_k F, \; F \in D(\bar{\Psi}_k) \right\}.$

Then for each k the composite mapping

(35) $\qquad \bar{\Psi}_k : D(\bar{\Psi}_k) \subset \mathfrak{F}_k(K) \to \bar{\mathfrak{F}}_k(K_d), \quad \bar{\Psi}_k = \Phi_k \Psi_k,$

will be called a __complete discretization mapping__ on $\mathfrak{F}_k(K)$.

Given K, K_d and Φ_k, the mapping $\bar{\Psi}_k$ gives a rigorous description

of the discretization process for a subclass $D(\bar{\Psi}_k)$ of operators in

$\mathfrak{F}_k(K)$. The following theorem then contains a commutativity result

analogous to Theorem 1:

Theorem 2: For k=1, 2, let $\bar{\Psi}_k : D(\bar{\Psi}_k) \subset \mathfrak{F}_k(K) \to \bar{\mathfrak{F}}_k(K_d)$ be complete

discretization mappings as in Definition 4. If $F = KG \in D(\bar{\Psi}_1)$ and

$G \in Q'(X,Z)$, then $F' \in D(\bar{\Psi}_2)$ and

(36) $\qquad\qquad (\bar{\Psi}_1 F)' = \bar{\Psi}_2 F' \qquad \text{on } \varphi_2(D(F')).$

<u>Proof:</u> $\Psi_1 F \in D(\Phi_1)$ since $F \in D(\bar{\Psi}_1)$, and applying Theorem 1 to $\Psi_1 F$ we have

$$(\bar{\Psi}_1 F)' \equiv \Phi_1 (\Psi_1 F)' = \Phi_2 (\Psi_1 F)' \quad \text{on } \varphi_2 (D((\Psi_1 F)')).$$

But $D((\Psi_1 F)') = D(F')$ and by Lemma 3, $(\Psi_1 F)' = \Psi_2 F'$. Altogether therefore

$$(\bar{\Psi}_1 F)' = \Phi_2 \Psi_2 F' = \ddot{\Psi}_2 F' \quad \text{on } \varphi_2 (D(F')).$$

Let us next consider composite operators of the form $F = GL$ where G is again some non-linear operator and L is a bounded and linear mapping. The differential operator (13) of Example 2 has this form, as can be seen if we introduce $W = C[0,1] \times C[0,1]$, define $L \in E(X,W)$ by $Lx = (x,x'')$ and let $G:D(G) \subset W \to Y$ be given by $G(w_1,w_2)(s) = f(s,w_1(s),w_2(s))$.

For operators of the form $F = GL$ we can proceed in a completely analogous manner as before, but some caution is necessary with respect to the definition of the domains of the operators. For the sake of clarity, this slight complication prompted the separate treatment of the two types of operators. It will be readily apparent how the theory can be formulated for more general operators, e.g., of the type $F = KGL$.

In general, let W be any Banachspace. For each $L \in E(X,W)$ define the linear operators $L_k \in E(X^k,W^k)$ by

$$(38) \qquad L_k(x_1,\ldots,x_k) = (Lx_1,\ldots,Lx_k) \qquad (k=1,2,\ldots),$$

and the operator classes

(39) $\quad \mathcal{G}_k(L) = \left\{ F \in Q(X^k,Y) \mid F = GL_k, \quad G \in Q(W^k,Y) \right\}.$

Note that $GL_k \in \mathcal{G}_k(L)$ only if $D(G) \cap L_k X^k$ is not empty.

As before, we introduce for any two L, $L_d \in E(X,W)$ the mapping

(40) $\quad \Psi_k : D(\Psi_k) \subset \mathcal{G}_k(L) \to \mathcal{G}_k(L_d), \quad \Psi_k(GL_k) = GL_{d,k},$

where

(41) $\quad D(\Psi_k) = \left\{ F = GL \in \mathcal{G}_k(L) \mid D(G) \cap L_{d,k} X^k \text{ not empty} \right\}$

and call Ψ_k a <u>pre-discretization mapping</u> on the subclass $D(\Psi_k)$ of operators of $\mathcal{G}_k(L)$. Note that here the pre-discretization mapping is no longer defined on the entire operator class $\mathcal{G}_k(L)$ as was the pre-discretization Ψ_k of Definition 3 for the class $\mathfrak{I}_k(L)$.

Corresponding to Lemma 3 we then have:

<u>Lemma 4:</u> For given L, $L_d \in E(X,W)$ and $k=1,2$ let $\mathcal{G}_k(L)$, $\mathcal{G}_k(L_d)$ and Ψ_k be defined as in (39) and (40). Let $F = GL \in D(\Psi_1)$, where $G \in Q'(W,Y)$, and assume that

(42) $\quad D_0 = \left\{ x \in X \mid Lx \in D'(G), \quad L_d x \in D'(G) \right\}$

is not empty. Then $F' \in D(\Psi_2)$ and

(43) $\quad (\Psi_1 F)' = \Psi_2 F' \text{ on } D_0 \times X$

<u>Proof:</u> For $x = (x_1, x_2) \in D_0 \times X$ we have by definition that $L_2 x \in D(G')$ and by the chain rule that $F' = (GL)' = G'L_2$. Hence $F' \in \mathcal{G}_2(L)$ and, moreover, $F' \in D(\Psi_2)$ since $D(G') \cap L_{d,2} X^2$ is not empty. Hence, for all $x \in D_0 \times X$

$$(\Psi_1 F') = (GL_d)' = G'L_{d,2} = \Psi_2(G'L_2) = \Psi_2 F'.$$

As before, we consider now the Φ-discretization mappings Φ_k, and for each k define the classes of operators

$$(44) \qquad D(\overline{\Psi}_k) = \left\{ F \in D(\Psi_k) \mid \Psi_k F \in D(\Phi_k) \right\},$$

and

$$(45) \qquad \overline{G}_k(L_d) = \left\{ \overline{F} : D(\overline{F}) \subset \overline{X}^k \to \overline{Y} \mid \overline{F} = \Phi_k \Psi_k F, \; F \in D(\Psi_k) \right\}.$$

Then the mapping

$$(46) \qquad \overline{\Psi}_k : D(\Psi_k) \subset G_k(L) \to \overline{G}_k(L_d), \qquad \overline{\Psi}_k = \Phi_k \Psi_k,$$

shall again be called a <u>complete discretization mapping</u> for the class $D(\overline{\Psi}_k) \subset G_k(L)$.

In analogy with Theorem 2 we now obtain

<u>Theorem 3:</u> For k = 1,2, let $G_k(L)$, Ψ_k, $D(\overline{\Psi}_k)$ and $\overline{\Psi}_k$ be defined as in (39), (40), (44) and (45). Suppose that $F = GL \in D(\overline{\Psi}_1)$ and assume that the set D_0 of (42) is not empty. Then $F' \in D(\overline{\Psi}_2)$ and

$$(47) \qquad (\overline{\Psi}_1 F)' = (\overline{\Psi}_2 F') \quad \text{on } \varphi_2(D_0 \times X)$$

<u>Proof:</u> From Lemma 4 it follows that $F' \in D(\Psi_2)$ and that $(\Psi_1 F)' = \Psi_2 F'$ on $D_0 \times X$. Since $F \in D(\overline{\Psi}_1)$ implies that $\Psi_1 F \in D(\Phi_1)$, we then obtain from Lemma 2 that $(\Psi_1 F)' \in D(\Phi_2)$ and therefore that $\Psi_2 F' \in D(\Phi_2)$.

Hence $F' \in D(\bar{\Psi}_2)$. But by Theorem 1

$$(\Phi_1(\Psi_1 F))' = \Phi_2(\Psi_1 F)' \text{ on } \varphi_2(D(\Psi_1 F)') = \varphi_2(D_0 \times X)$$

and this completes the proof.

As mentioned before, it is now simple to combine Theorems 2 and 3 to obtain corresponding results for operators of the type KGL, e.g., for integro-differential operators of the form (21), and for more general composite operators. Another simple generalization gives results for higher order derivatives. We shall not detail these generalizations here.

5. Application to Newton's Method

In this Section we return to the observation mentioned in the Introduction that discretization and Newton's method "commute". The results obtained in the previous sections now allow a precise formulation of this observation.

For the sake of simplicity, let us restrict ourselves to the class of operators $\mathfrak{F}_1(K)$ defined in (31), i.e., operators of the type $F = KG$. Let $F \in D(\bar{\Psi}_1) \subset \mathfrak{F}_1(K)$ and $\bar{\Psi}_1 F = \bar{F}$. As in the Introduction, we define the "Newton"-functions of F and $\bar{F}$ by

(48) $$N(x,y) \equiv F'(x;y) + F(x),$$

and

(49) $$\bar{N}(\bar{x},\bar{y}) \equiv \bar{F}'(\bar{x};\bar{y}) + \bar{F}(\bar{x}),$$

where evidently $D(N) = D(F')$ and $D(\bar{N}) = D(\bar{F}')$. Then the following

theorem states that on $\varphi_2(D(F'))$ the complete discretization of the Newton function N of F coincides with the Newton function of the complete discretization $\bar{F}$ of F. This is the precise meaning of the "commutativity" of Newton's method and discretization.

<u>Theorem 4:</u> Suppose $F \in \mathfrak{F}_1(k)$ satisfies the conditions of Theorem 2. Let $\bar{F} = \bar{\Psi}_1 F$ and consider the Newton functions N and $\bar{N}$ as defined by (48) and (49), respectively. Then $N \in D(\bar{\Psi}_2)$ and

(50) $$\bar{\Psi}_2 N = \bar{N} \text{ on } \varphi_2(D(F'))$$

<u>Proof:</u> By assumption, $F \in D(\bar{\Psi}_1)$. If F is considered as a function on X^2, i.e., $F(x_1,x_2) \equiv F(x_1)$, then also $F \in D(\bar{\Psi}_2)$. Moreover, from Theorem 2 it follows that $F' \in D(\bar{\Psi}_2)$ and that $(\bar{\Psi}_1 F)' = \bar{\Psi}_2 F'$. Using the fact that $\bar{\Psi}_2$ is linear on $D(\bar{\Psi}_2)$ we have for $x,y \in D(F')$

$$(\bar{\Psi}_2 N)(\varphi x,\varphi y) = (\bar{\Psi}_2 F')(\varphi x; \varphi y) + (\bar{\Psi}_2 F)(\varphi x)$$

$$= (\bar{\Psi}_1 F)'(\varphi x; \varphi y) + (\bar{\Psi}_1 F)(\varphi x)$$

$$= \bar{N}(\varphi x, \varphi y)$$

or

$$\bar{\Psi}_2 N = \bar{N} \quad \text{ on } \varphi_2(D(F))$$

and this completes the proof.

Clearly the principal reason for the validity of this theorem is the linearity of N in terms of F and F' and the "commutativity" of discretization and differentiation. Accordingly, the result can be readily extended to any linear combination of a function and its derivatives. We shall not go into details here.

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